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Accuracy and Limits of Applicability of Solutions of Equations of Transport; Dilute Monatomic Gases

HAROLD GRAD

September 30, 1964

AEC Research and Development Report

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ACCURACY AND LIMITS OF APPLICABILITY OF SOLUTIONS OF EQUATIONS OF TRANSPORT; DILUTE MONATOMIC GASES

Harold Grad

I. Introduction

We consider the theory of the Boltzmann equation for a simple gas of monatomic molecules. This has the most highly developed theory and should serve as a prototype for the ultimate development of more complex equations governing dense gases, molecules with internal structure, plasmas, etc. Mixture of gases, although presenting much more complicated bookkeeping and entirely different physical phenomena, offer no new mathematical problems.

We shall be concerned more with a survey of general methods and principles than with summarizing solutions to specific problems. The reason is two-fold. First there is the danger of improper extrapolation from isolated special solutions without qualitative guidance from a general theory; second there is the vital question whether the equations have any meaning, which is never answered by any number of special solutions. Except in cases where there is a very well-developed theory (e.g., Laplace's equation), we must pursue two paths simultaneously: an investigation of whether the equations are intrinsically meaningful, and the pursuit of

results which can be used to interpret physical phenomena. Although there have been very significant recent advances in general theory, there is still a large class of problems where it is not known whether the Boltzmann equation formulation makes sense (note, this caution applies even to problems of monatomic perfect gases).

Specifically, this report brings up-to-date the similar surveys contained in the author's articles in the Handbuch der Physik (1958) and in the proceedings of the Nice Symposium (1958). The principal advances since that time (in addition to some significant special solutions*) are a more comprehensive knowledge of the theory of the linearized Boltzmann equation[3] and a better appreciation of the two singular extremes, the approach to free flow[4,5] and the approach to a classical continuum[6,20].

There is a very large choice of equations that can legitimately be called "the" Boltzmann equation as well as a number of model equations, chosen primarily for their mathematical convenience. Although many of the distinctions might be termed slight on physical grounds (e.g., use of a cutoff potential instead of an infinite range but rapidly decaying potential), it is an unfortunate fact that the mathematical nature of the equations, and even more, the

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* References 4, 5, 14, 15, 16, 21, 22.

success of a given approximation procedure, is extremely sensitive to the precise formulation of the problem. Thus the success of a given formulation of the Boltzmann equation, or of a given approximation technique, is much more closely dependent on the mathematical structure than on the physics. There is always the question of the value of an equation that is too difficult to solve; but there is also the more subtle question, whether an equation has any solutions at all. One can find equations suggested by very plausible physical arguments which are utterly meaningless and do not have any solution at all. By being "approximate", one can find and even publish "practical" information from such meaningless equations; the fault lies in an automatic filter which discourages publication of nonsensical results, but not plausible results obtained by nonsensical means.

Restated, the validity of a given system must be evaluated in two independent ways; by verifying the existence and uniqueness of solutions, continuous dependence, etc. The need of a general theory is not only to establish that the system has meaning and is worth considering further, but also to avoid the pitfall of extrapolating from possibly nonrepresentative special cases. We mention a few examples.

(1) The special solution obtained by Ikenberry and Truesdell[7] for heat flow is the only explicit solution (other

than the trivial Maxwellian) that is known for the nonlinear Boltzmann equation. But, after development of a comprehensive theory of the linear equation, it is found that the conclusions that were drawn on the basis of this explicit solution are completely misrepresentative of the general case.[6]

(2) Another example exhibits many solved problems, all of which are nonrepresentative. Use of the Navier-Stokes equations (with a slip boundary condition where necessary) gives fairly good results for sound dispersion over all measurable wavelengths, very good results for the shock profile for virtually all strengths, excellent results for Couette flow or heat flow (parallel plates or concentric cylinders) for <u>all</u> values of the mean free path. It yields nonsensical results for virtually all other geometries in the limit of large mean free path (viz., finite drag in a vacuum), but there is only one case simple enough to show this analytically, flow around a sphere![23]

(3) Finally, the discrete spectrum of the collision operator for Maxwell molecules exploited so successfully by Uhlenbeck[8] and others[9,10] has recently been found to be very special.[3] The significance of the existence of a continuous spectrum has still to be exploited.

II. Various Formulations of the Boltzmann Equation and their Accessibility to Theory.

The term "Boltzmann equation", even when restricted to the classical equation of the theory of monatomic simple gases, is at least as broad a concept as say "Fredholm integral equation" or "elliptic differential system", and efficient techniques for solution must be tailored to the specific intermolecular potential and problem. Any method which does not make such distinctions is likely to be a crude one.

For example, hard potentials (harder than Maxwellian) yield an unbounded collision frequency for fast particles, while soft potentials(softer than Maxwellian) exhibit a collision frequency that approaches zero for large velocity. A crude experimental result, or even a crude theory may be insensitive to this difference. But any precise handling should take into account that the tail of the distribution is in one case almost instantly equilibrated and in the other case acts almost independently of the rest of the gas. We can say that the effective Knudsen number of the tail is either very large or very small compared to that of the bulk of the gas. Mathematically, this is reflected in the fact that the linear collision operator has a continuous spectrum, in one case extending from a finite value to infinity, in the other, from

a finite value to zero.[3] In the latter case, for example, one cannot expect uniform exponential decay to equilibrium. Even if such distinctions can be safely neglected physically, they cannot be neglected mathematically. At the present time, the presence of the continuous spectrum has been exploited only negatively, to cast doubt on certain accepted approximation procedures (one exception is ref. 14 where the continuum is explicitly treated).

With reference to the mean free path (relevant in steady flow), the case of hard spheres must be distinguished from all other softer potentials for which the mean free path vanishes for high velocity.

The rigorous solution of any nontrivial problem with an infinite total cross section has thus far eluded our grasp (this statement even includes the case of Maxwellian molecules for which the spectrum is discrete and the eigenfunctions explicit). Even for cutoff potentials, although a cutoff in angle of deflection (grazing deflections) yields a mathematically tractable equation[3], a cutoff in physical space (i.e., impact parameter) has not yet yielded to any substantial theory. It is an open question whether the infinite cross section (which yields a collision integral which is not absolutely integrable) merely makes the problem mathematically

difficult, or whether the equation itself is a poor one.

With regard to the nonlinear equation, it is claimed in several places in the literature that one should not expect an equation of this type to have solutions in the large[11,12] (we do not hold with this opinion), and several modifications of the classical equation[11,12] have been put forth as replacements (these are not the so-called model or single-relaxation equations which would be subject to the same doubts).

With regard to the use of model equations we first mention two competing principles:

(1) any equation which can be solved is more useful than one which cannot be solved, no matter how much "better" the second one is on physical grounds.

(2) a more primitive equation loses its interest when it becomes possible to solve comparable problems with a more sophisticated equation. In Ref. 1. it is stated that a relaxation model equation is useful when linearized, only provided that one can exploit Fourier analysis as a tool, and in the nonlinear case only when solved numerically (which is virtually impossible for a true Boltzmann equation). The first region of application has lost some of its attraction because of the development of the theory of the linear Boltzmann equation (with cutoff potentials). For boundary value

problems[13,14,5,15] and nonlinear problems[16], the model equations still retain their value.

III. Linear Theory

A comprehensive theory of the initial value problem for quite general cutoff repulsive potentials, has been obtained.[3] These strengthen and generalize results due to Carleman[17]. In particular, for the equation

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla f + L[f] = 0, \tag{3.1}$$

under a specular boundary condition, the initial value problem has been shown to be well posed. The solution exists, is unique, smooth, bounded, well-behaved in velocity space, and decays to equilibrium as $t \longrightarrow \infty$. The growth estimates are nontrivial because they include fluid flow as a special case (small mean free path), and we need only call attention to a spherical implosion which may yield very large perturbations at a later time (even in the linear theory). This theory includes as special cases all single or multiple relaxation models of the Boltzmann equation, including velocity-dependent collision frequency; some of these have also been studied using Fourier transform[18]. The decay to equilibrium (H-theorem)*

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* H. Grad, "On Boltzmann's H-Theorem", to be published in Proc. of the SIAM von Karmann Symposium, Washington, D.C., May 1964.

is the only part that requires separate treatment for soft and hard potentials. It is worth noting that the decay to equilibrium involves a complicated interplay between decay to an approximate local Maxwellian (usual H-theorem) and viscous decay due to a residual small deviation from Maxwellian.

A simpler equation is the spatially homogeneous one

$$\frac{\partial f}{\partial t} + L[f] = 0. \tag{3.2}$$

The behavior of the solutions depends on the spectrum of the operator L (which is singular and unbounded in general). For almost all potentials, L has a continuous spectrum. For hard potentials, the continuum extends to infinity (Fig. 1a); for soft potentials to the origin (Fig. 1c). For a cutoff Maxwellian (constant collision frequency), there is a discrete spectrum with a finite accumulation point (Fig. 1b).

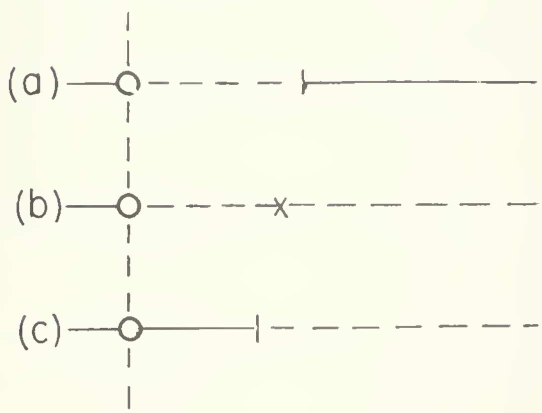


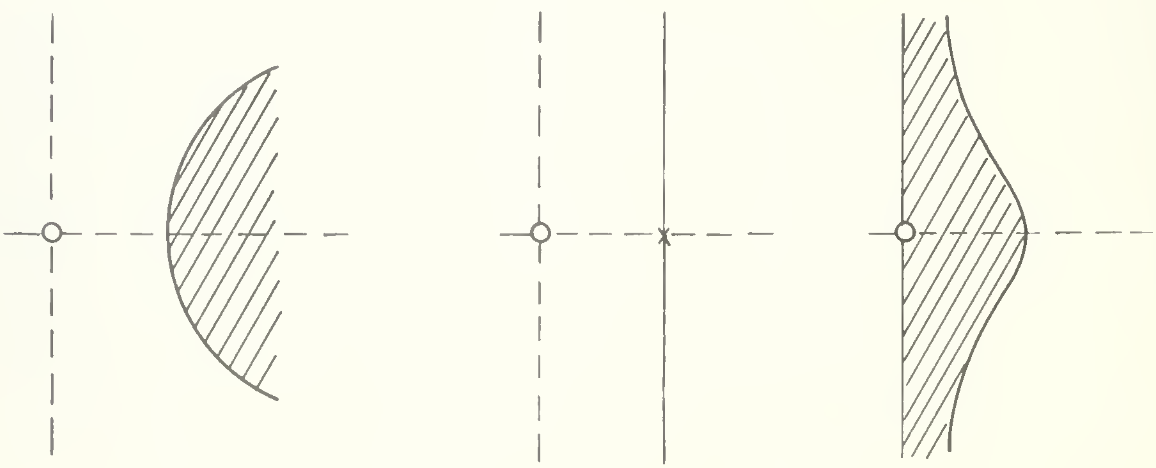
Fig. 1

There exists a complete set of normal modes only for the Maxwellian. There is a uniform exponential decay to equilibrium only for a hard potential.

In between (3.1) and (3.2) in difficulty, we can look for solutions of (3.1) which are harmonic in their space dependence

$$\frac{\partial f}{\partial t} + i\xi \cdot kf + Lf \equiv \frac{\partial f}{\partial t} + \mathcal{L} f = 0 \; . \tag{3.3}$$

As in (3.2), the behavior of the solutions depends on the spectrum of $\mathcal{L} = i\xi \cdot k + L$. For a cutoff Maxwellian, the continuous spectrum is a line parallel to the imaginary axis (Fig. 2b); for a hard potential it is the area to the right of a certain curve (plausible conjecture), and for a soft potential it is a region between the axis and a certain curve (plausible conjecture). Thus in no case (even the Maxwellian) are there enough normal modes [i.e., complex values of ω which permit solution of $(i\omega + i\xi \cdot k)f + Lf = 0$] for given fixed k, to solve an initial value problem. Furthermore, for sufficiently large k, there are probably no normal modes, and the asymptotic behavior for large t is not exponential.



(a) (b) (c)

For soft potentials, there are no isolated normal modes for any value of k. For a pure boundary value problem (e.g., heat flow)

$$\xi \cdot \nabla f + L[f] = 0 \tag{3.4}$$

or wave propagation from an oscillating wall

$$i\omega f + \xi \cdot \nabla f + L[f] = 0, \tag{3.5}$$

one can give plausible arguments that indicate that the continuum extends to the origin in all cases except the hard sphere. There may be a limited number of normal modes, but the asymptotic behavior far from the wall will arise from the continuum and will not be a simple exponential decay (except possibly for the hard sphere).

For non-cutoff potentials, we cannot even begin to guess at the spectrum of L because in the one case for which it is known (Maxwellian), if we introduce a cutoff approximating potential, we are exactly at the borderline case of a continuum which extends either to the origin or to infinity, and the initial point of the continuum moves off to infinity with the cutoff.

The nature of the spectrum of $\mathcal{L} = L + i\xi \cdot k$ for the non-cutoff Maxwellian does not seem to follow from any known

theorems, but it could conceivably be a pure point spectrum, even though for the cutoff Maxwellian $\mathcal{L}$ there is a continuum.

Although the theory of the linear Boltzmann equation is advancing rapidly, the most significant practical consequence, thus far, is to cast doubt on the most common method of approximation (viz. polynomial expansions and the concomitant exponential dependence). Such expansions can only be interpreted as ad hoc approximations which may yield rough answers but do not reflect the correct analytic properties of the solution.

IV. Dependence on the Knudsen Number

The essential significance of the Boltzmann equation lies in the solution of problems in which the mean free path is finite compared to other relevant dimensions. Thus problems in free flow and the computation of transport coefficients can both be considered trivial uses of the Boltzmann equation. On the other hand, the transition to gas dynamics are in both cases highly singular, and these transitions must be understood throughly before we can hope to use more than ad hoc measures in the intermediate range.

With regard to the computation of transport coefficients using the Boltzmann equation, the problem is very well understood, except that actual computations for a specific potential which is not monotone may be very lengthy, and the bookeeping for a

mixture of gases may be very elaborate. The theory of the integral equation which has to be solved in the Chapman-Enskog theory is not nearly so sensitive to variation in molecular potential as is the Boltzmann equation itself.

With regard to free flow, the equation itself is trivial, but in complicated domains, one faces substantial, but well-understood problems involving conventional types of integral equations[19].

The approach to free flow is characterized by singular behavior, at least for plane Couette and plane heat flow, because of the existence of a class of particles which is dominated by collisions no matter how large the Knudsen number is (almost grazing to the plate)[4]. This is reflected in a heat transfer or drag which depends logarithmically on the Knudsen number. Presumably, the logarithm will enter at a higher order term for a cylindrical problem where the class of exceptional particles is smaller.

Another problem in which it is not certain that the limit is singular is flow around a body (e.g., a sphere)[5]. There is always a large class of particles which is collision-dominated, viz., all those farther than a mean free path from the object. But, since the immediate neighborhood of the object is uniformly in free flow, it is not surprising that the first order perturbation in drag is regular in K, but

it is an open question whether the dependence will remain regular to higher order. One would expect, similarly, that if there is any singular behavior in a spherical Couette or heat flow, this also will take a more subtle form.

The approach to a continuum is much more singular, as evidenced by the reduction from a description in terms of fluid variables. This problem has received considerable attention recently, and is summarized in the next section.

For the intermediate case of finite Knudsen number, there is no general theory, and we can only use the limiting cases of small and large mean free path as guides for the suggestion of plausible techniques; similarly, we may, with caution, use the relatively complete linear theory as a guide for the solution of nonlinear problems. This will be discussed in the concluding section.

V. The Approach to Fluid Dynamics

Hilbert's theory is obtained by formally substituting a tentative expansion

$$(5.1) \qquad F_H(\xi,x,t) = \sum_{0}^{\infty} \varepsilon^n f_H^{(n)}$$

into the Boltzmann equation with a parameter ε (mean-free-path scaling factor)

(5.2) $$\frac{\partial f}{\partial t} + \xi \cdot \nabla f = \frac{1}{\varepsilon} J(f,f),$$

and equating coefficients of powers of ε. A formal result of substituting this series is that f_H is uniquely determined as a function of ξ by the instantaneous values of the fluid state. The Chapman-Enskog method adopts this uniqueness theorem as a postulate, and provides an algorithm for determining f_H term by term in terms of the fluid state. This is a mysterious result, since the Boltzmann equation (5.2) can be assigned an arbitrary initial f which is not equal to any f_H.

This mystery has been resolved[6,20] by showing the existence of a different formal expansion

(5.3) $$f_\mu = \sum_0^\infty \varepsilon^n f_\mu^{(n)}$$

which also formally satisfies the Boltzmann equation term by term, but it is uniquely determined by the <u>orthogonal complement</u> to the fluid state, and also decays exponentially in a time of order ε. An arbitrary initial function $f(\xi,x,t)$ can be uniquely decomposed into a sum $f_H + f_\mu$. The component f_μ carries a nonvanishing fluid contribution. Therefore, the correct Hilbert function f_H does not carry the entire fluid state. In other words, the tacit assumption in the Hilbert

and Chapman-Enskog theories, that the parameters which occur naturally are to be identified with the fluid state, is incorrect. The interference between f_μ and f_H allows us to compute the correct initial values that must be used in the Chapman-Enskog theory (not the fluid state) in order for f_H to be correctly asymptotic to the exact solution after f_μ decays.

These results have been obtained formally for the nonlinear Boltzmann equation and rigorously (the series are shown to be asymptotic to true solutions of the Boltzmann equation) for the linear equation (with cutoff hard potentials)[6]. The ε expansions are truly asymptotic in that it can be shown that they are convergent only in very special nonphysical cases. As a consequence the Burnett and higher order approximations are only useful as improvements when the Navier-Stokes equations are already good; they do not serve to extend fluid dynamics further into the slip-flow regime.

This result solves one of three connection problems posed in Ref. 1 for the, presumed asymptotic, Chapman-Enskog series. In addition to supplying correct asymptotic initial data, one must supply correct asymptotic boundary data and correct jump conditions across any shocks which occur (the expansion is clearly invalid in these three layers of nonuniform convergence). Descriptive terms for these three problems are

initial slip, boundary slip, shock slip. The boundary slip problem is classical (Maxwell), but no accurate results are known except for one in the special case of shear flow using a model equation by Cercignani[14]. An approximate solution has also been given in a special case of the shock slip problem by Pan and Probstein[21]. But the problems of determining boundary conditions and jump (Hugoniot) conditions to complete the Hilbert-Chapman-Enskog theory are still to a large extent open.

Another question which is entirely unanswered at the present time is whether the higher order systems arising in the Chapman-Enskog theory (e.g., the Burnett equations) are meaningful. It is known that similar procedures for the f_μ rather than the f_H can lead to meaningless equations at times.[6]

Although the usefulness of higher order Chapman-Enskog terms in solving flow problems is strictly limited, the values of transport coefficients as ordinarily computed are absolutely correct.

VI. Critique of Methods

Probably the most widespread method of solving problems using the Boltzmann equation is to approximate the distribution function by a selected sum of definite functions of velocity with undetermined "macroscopic" multipliers depending on x and t.[24] As a strict expansion in eigenfunctions, this, we

have seen, has very restricted validity. On the other hand, as an *ad hoc* approximation scheme it may give good overall results while hiding subtle analytic dependences. In linear problems there is hope of doing better, once the analytic nature of the relevant operators is fully exposed. In nonlinear problems, there is little hope of a comprehensive general theory in the near future, so *ad hoc* methods cannot be dismissed. The crucial point in such a procedure is to be clever in selecting the approximation functions to fit the special problem that is at hand. For example, one must balance the awkwardness of half-range expansions (or worse, in non-plane geometries) against their better fit in the large Knudsen number regime. A good example of accurate fitting is Ref. 22.

One must use care in obtaining "moment equations" which govern the undetermined macroscopic variables. For example, hyperbolic equations allow the use of a much more well-developed theory than parabolic equations but they may have more of a tendency to break down in nonlinear problems[1]. We must refer again to the unfortunate mathematical fact that the success of a plausible approximation in such uncharted regions is very hard to predict *a priori*.

We include in this *ad hoc* category the bimodal distributions that have been used to evaluate shock profiles, although there seems to be a superstition prevalent that a bimodal distribution is in some sense *correct* for a strong shock.

A more specialized (but still quite general) technique is integral iteration. This has the simultaneous advantage and disadvantage of the built-in exponential convergence factor. One can interpret this iteration as advancing a correction roughly one mean free path or one mean collision time per iteration. It is therefore very good if the entire domain is smaller than a mean free path. It is also very good if the initial approximation, thought of as an initial value, would converge to the correct steady solution within a few collision times (this is probably the reason for the success of the numerical solution of the shock profile for a model equation[16]). But a great disadvantage is the (usual) impossibility of doing more than a single iteration analytically. Integral iteration is also a very useful tool for purely theoretical (not necessarily constructive) investigations. One iteration is a good approximation where most particles move from one wall to another with only a small probability of collision, but it is only a rough estimate in other almost free flow problems (e.g. flow around a small sphere).

One might suspect that an optimum "engineering" solution of a problem, minimizing the effort/result, would be to take some low level analytic solution obtained by polynomial (or other) approximation of the distribution function, and follow this by a numerical iteration. This would have the advantage

of starting the iteration with an approximate fit which exhibits parameter variations explicitly.

We conclude with a reiteration of the statement made in Ref. 1 that the problems that appear to be solvable by these techniques are still far from being exhausted. But, since we are beginning to discover some of the underlying mathematical structure, it may soon be possible to use more effective and specifically appropriate methods rather than brute force in some areas.

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